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20. ABSTRACT

Two fundamental problems involved in the hetero-epitaxial growth of GaAs on Si substrates were investigated: (a) The mechanism by which antiphase domain disorder is self-eliminating under proper growth conditions. (b) The minimization of misfit-induced threading dislocations, and the properties of those dislocations that remain, especially their interactions with superlattice buffer layers.

Although the self-elimination of antiphase domain disorder under proper growth conditions is experimentally beyond the shadow of a doubt, no truly satisfactory explanation for this (desirable) phenomenon has been found. All explanations proposed so far fly in the face of at least some experimental data. In fact, some of the experimental data fly in the face of each other. We propose that the self-elimination is of kinetic rather than energetic origin, and that the details of the annihilation mechanism depend sensitively on details in the kinetics. The apparent conflicts between some of the experimental data themselves are presumably due to differences in the kinetics employed by different investigators.

Contrary to a widely-held belief, superlattice buffer layers are only marginally effective in reducing threading dislocation densities of the magnitude occuring in GaAs-on-Si growth, and they are unable to reduce the densities to anywhere near the levels desirable for the more demanding device applications, such as lasers. Repeated high-temperature anneals during growth are about one order of magnitude more effective, but a truly satisfactory level of dislocation reduction will probably require island-like growth on patterned substrates.

Threading dislocations were found interact strongly with superlattices, in a way that superficially suggests that non-radiative recombination at dislocations has been suppressed. If true, this would be a most desirable phenomenon. However, the effect was traced to a reduction in the mobility of the minority carriers *along* the superlattice wells, presumably caused by dislocation-induced well width fluctuations. This causes the minority carriers to be effectively trapped in regions of enhanced well width, where they recombine radiatively before reaching he dislocation.

Molecular Beam Epitaxial Growth & Electronic Properties of GaP-on-Si (211) Heterostructures, and of Related Systems

Final Report

by

Herbert Kroemer

November 1990

U. S. Army Research Office

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DAAG29-85-K-0107

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REPORT ON THE RESEARCH

A. The Problems

The research conducted under this contract was a follow-up to research conducted under two earlier ARO contracts (DAAG29-77-C-0041 and DAAG29-81-K-0143) under the title '*Molecular-Beam Epitaxial Growth and Device Potential of Polar/Nonpolar Semiconductor Heterostructures.*' Under those earlier contracts, we had succeeded in the first high-quality growth of any III/V compound on a column-IV elemental semiconductor, specifically the growth of GaP on Si.[1,2] In fact, not only had we achieved the growth of high-quality GaP layers per se, but the GaP/Si hetero-interface itself was of sufficient quality to permit the demonstration of a working heterostructure bipolar transistor with a GaP emitter on a Si base/collector structure, in which the GaP/Si interface was actually located inside the device structure proper, right at the most defect-sensitive location inside the device, the emitter/base interface. The achievement of such device-internal interfaces had been one of the explicit goals of that research.

Two of the 'secrets' behind that success had been the use of GaP rather than the more interesting GaAs as the III/V compound, and the use of the previously unused (211) crystallographic orientation rather than the almost-universally used (100) orientation.

The reason for the choice of GaP was our conviction that a close lattice match between the compound semiconductor and the Si substrate would be necessary not only for acceptable bulk quality of the epi-layer, but would be absolutely essential for a low-defect device-internal interface. This naturally led to the reasonably well lattice-matched pair GaP-on-Si (mismatch 0.4%), at least for the initial work, rather than GaAs-on-Si, with a lattice mismatch ten times as high (4%).

The reason for the choice of the crystallographic (211) orientation had been our own discovery that the crystallographic (211) plane assured epitaxial growth free of antiphase disorder, a condition believed necessary for the growth of device-quality layers. As may be recalled, the antiphase domains problem is that of random domains containing opposite assignments of the lattice positions to the Ga and P atoms. We were — and are — convinced that any III/V compound semiconductor film containing APDs would be useless for true device-quality material.

As the title of the proposal for the research reported here indicated, it was originally intended to follow up the (211)-oriented GaP-on-Si work, with GaAs-on-Si work (the 'related systems' in the title of the proposal) being a secondary objective. However, by the time the new contract actually got underway, a major new priority had arisen for both ARO and ourselves: the development of a GaAs device technology using Si rather than GaAs substrates.[C 1]* It is important to realize that this shift was *not*

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1 S. L. Wright, M. Inada, and H. Kroemer, J. Vac. Sci. Technol. **21**, 534 (1982).

2 S. L. Wright, H. Kroemer and M. Inada, J. Appl. Phys. **55**, 2916 (1984).

* References in this form, [C ...], are to papers published under this contract, listed in Sec. C of this Report

towards GaAs/Si heterojunctions with device-internal interfaces; the role of the Si was strictly that of a substrate, with the GaAs/Si interface far removed ($\geq 1\mu m$) from the device structure proper. In fact, it was clear from the beginning that there was no hope to achieve GaAs/Si interfaces of sufficient quality to permit their incorporation into the device structures proper.

In a sense, this abandonment of the requirement that the GaAs/Si interface be part of the device proper, made the problem substantially easier than our original objective of making device-internal polar/nonpolar interfaces. At the same time, the problem was made substantially harder by the much greater lattice mismatch in the new materials combination, which was expected to dominate the problem — and did.

We anticipated at the outset that many others would also engage in research on GaAs-on-Si technology, but that most of them would probably concentrate on actually demonstrating finished devices, rather than addressing themselves to the scientific understanding of the two defect problems, antiphase domains and threading dislocations. We therefore deliberately concentrated our own work on those defect aspects, the solution of which we felt — and feel — is essential to long-term progress.

B. Summary of Results.

a) The Antiphase Domain Disorder Problem.

Through our earlier work under the predecessor contracts, we had been acutely aware of the antiphase disorder problem in polar-on-nonpolar growth. Like some others working on this problem, we had been convinced — erroneously, it turned out — that APD-free growth was fundamentally unachievable on (100)-oriented wafers, with their inevitable surface steps. Having ourselves shown that the problem is truly absent in (211)-oriented growth, we naturally continued to pursue the (211) approach [C 1-3].

Others, not persuaded by our theoretical arguments, and disinclined to use the unconventional (211) orientation, continued to work with (100) or near-(100) wafers. By mid-1985, several groups had presented convincing evidence that it was indeed possible to grow GaAs epi-layers on slightly misoriented (2°-4°) Si (100) substrates in such a way that at least the upper portion of sufficiently thick ($> 1\mu m$) layers was demonstrably APD-free, even over wafer-sized areas.[3] It remained (and still remains) unclear whether the growth is already nucleated APD-free, or one of the two possible domain orientations overwhelms the other as the growth progresses.

To the extent that the various investigators offered explanations for the mechanism at all, these initial *explanations* were all untenable, without a single exception. But that did not invalidate the results themselves.

With the achievement of APD-free (100) growth, our (211) approach became less interesting, and our own research on the APD problem shifted towards *understanding*

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[3] For detailed references, see paper [C 3]

how mis-oriented (100) growth could either start truly APD free, or at least how a *perfect* mutual annihilation of any initially present APDs could take place as the growth progressed Much of this work involved us in refuting various existing but untenable "explanations."

In 1986 it appeared that we had found the mechanism [C 3,5,6]. We pointed out that an APD-free *ab-initio* nucleation implied that *all* terraces on the misoriented Si starting surface belong to the same sublattice of the diamond structure of Si, rather than to alternating sublattices. Following up on an earlier suggestion by Kaplan,[4] we concluded that the driving force for such a preference could only reside in the energetics of the dangling bonds at the terrace edges. This energetics seemed to prefer the dangling-bond configuration of one of the two sublattices over that of another. The preference for one particular sublattice as the terrace surface implies a doubling-up of *all* surface steps, with one of the two possible sublattice sequences at the terrace edges preferred over the other, and over single steps. The desired step doubling-up presumably took place during the high-temperature 'heat-cleaning' stage that was employed in all successful growth recipes. Shortly after our work, Aspnes and Ihm[5] independently came to the same conclusion, and they actually postulated a certain reconstruction of the bonds at the double-step terrace edge as providing the driving force.

The model explained the then-existing data well, but it was soon refuted, when several authors showed conclusively that APD-free growth can be achieved even when the postulated double steps are demonstrably absent [C 9].

The puzzle was deepened by observations that Nature's preferred sublattice allocation for APD-free growth depended on the growth conditions,[6] such as growth temperature, whether the growth is started with an exposure to As or to Ga, and even on whether the As molecular species employed wasAs_2 or As_4. As it stands now, we are not aware of a satisfactory explanation for the full range of observed behavior, one that does not fly in the face of at least some of the empirical facts [C 12].

In fact, some of the raw empirical facts fly in the face of each other. For example, there are convincing experimental data that the growth becomes single-domain within a few (<10) monolayers, and equally convincing data that the disappearance of APD requires hundreds or thousand s of monolayers, both sets of data coming from first-rate experimentalists with impeccable credentials. Contradictions such as these suggest that maybe the kind of interface formed is not so much a matter of energetics as a matter of kinetics.

Towards the end of this contract, we had been led to this suspicion by different considerations, independently of those conflicting experimental observations. Practically alone amongst researchers in this field, we had long felt that questions of electrical neutrality at the interface play an important role in what atomic configuration forms. It is not difficult to show that an electrically neutral interface must contain an

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4 R. Kaplan, Surf. Sci. **93**, 145 (1980)

5 D. E. Aspnes and J. Ihm, Phys. Rev. Lett. **57**, 3054 (1986)

6 For detailed references, see papers [C 5,6,9, and 12]

equal number of Ga-Si and As-Si bonds. Any imbalance in those bonds will necessarily cause interface charges, with an accompanying electrostatic energy penalty. If this penalty is large enough, any energetic preference for one sublattice allocation over another would be diminished, and easily overridden by kinetic considerations. We firmly believe this to be the case in GaAs-on-Si epitaxy [C 12].

b) The Misfit-Induced Threading Dislocation Problem

With the antiphase domain disorder problem having faded from immediate urgency (without having really being solved), most of our own research — like that of others — focussed on the dislocation problem. We had of course been acutely aware of the fact that the 4% lattice mismatch between GaAs and Si was bound to lead to very large densities of in-plane misfit dislocations, many of which propagate into the epi-layer as threading dislocations — this had, after all, been the sole reason for working with GaP rather than GaAs in our earlier work. Although the in-plane misfit dislocations are clearly unavoidable for purely geometric reasons, there existed, at the time this contract got under way, a widely-held belief that the *threading* dislocations could be very effectively suppressed by superlattice buffer layers. Some of our own earlier work on GaSb/AlSb superlattices grown on GaAs substrates (8% mismatch!) seemed to support this belief: We had found that these superlattices exhibited excellent photoluminescence properties, suggesting that the inevitable threading dislocations had indeed been annihilated in the lower portions of the superlattice.[7]

This belief was shattered when we acquired an "everyday" transmission electron microscopy capability, which showed that the dislocation density was huge (> $10^7/\mathrm{cm}^2$), and that almost no additional dislocation annihilation had taken place beyond that achieved by simply growing the same thickness of material without a superlattice. Yet at the same time, it was clear that the non-radiative recombination efficiency of the dislocations had been reduced by orders of magnitude, presumably by the presence of the superlattice. The latter conclusion was also supported by the first published reports of GaAs/(Al,Ga)As lasers grown on Si substrates: All lasers that actually worked were narrow-well quantum well lasers, while ordinary double-heterostructure lasers failed dismally.

The solution of this puzzle was to form the core of our *experimental* research under this contract. The results of this research may be summarized as follows [C 11-13]:

> (1) The reduction of the non-radiative recombination efficiency of the threading dislocations is the result of a drastic reduction of the minority carrier *mobility* along narrow quantum wells, caused by potential fluctuations inside the wells. The minority carriers simply do not get to the dislocations, where they would recombine non-radiatively, but become trapped at local potential minima, where they recombine radiatively. This mechanism is not considered a viable mechanism for suppressing the deleterious effects of the threading dislocations.

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[7] G. Griffiths, K. Mohammed, S. Subbanna, H. Kroemer, and J. L. Merz, Appl. Phys. Lett. **43**,1059 (1983).

(2) Superlattice buffer layers are almost totally ineffective in suppressing the high native threading dislocation density near the GaAs/Si interface (> $10^{11}/cm^2$) to much below $10^7/cm^2$, a value still three orders of magnitude above what would be desirable for the most demanding application, lasers. They are only slightly more effective than doing nothing at all (other than just growing 1μm of ordinary GaAs and relying on natural dislocation annihilation), and they are much less effective than a simple periodic anneal during growth.

(3) Although we ourselves did not work with the periodic anneal technique, the published reports indicate that it, too, saturates at still-too-high dislocation densities around $10^6/cm^2$.

In an attempt to understand better whether there is a theoretical basis for these disappointing observations, we developed a simple model for the dislocation annihilation kinetics [C 12]. The model showed clearly that, once the dislocation density has dropped below about $10^8/cm^2$, the dislocations are simply too far apart to "find each other" and to recombine, over a reasonable thickness of subsequent growth. The reason the periodic anneal seems to work is that it greatly enhances the dislocation mobility, thereby effectively increasing the distance over which dislocations can interact. Our model also explains why the dislocation density does not decrease exponentially with growth thickness, but only by a simple inverse linear law. Repeated buffer layers do not act multiplicatively, but only additively. Finally, the model explains why the final dislocation density after a given growth thickness seems to be essentially independent of the initial dislocation density, once the combination of lattice mismatch and layer thickness exceeds the critical thickness combination beyond which the misfit dislocations form.

Probably the best hope to achieve a major and reduction in threading dislocation density, and perhaps even their complete elimination, lies in island-like epitaxial growth on suitably patterned substrates, during which the dislocations simply get pushed out of each island. Practically all devices of interest could be accommodated inside such islands, including lasers. We did not have the resources left to pursue this idea further, but we would recommend that any further research on GaAs-on-Si epitaxy be concentrated in this area.

Confronted with these negative conclusions, we decided to re-examine the question as to the possibility to simply "live with" dislocation densities around $10^7/cm^2$, and we came to some surprising conclusions [C 12]. It is often said that minority carrier devices, such as heterostructure bipolar transistors (HBTs) and solar cells, cannot tolerate such high densities. Upon a quantitative study of the problem we concluded that the statement holds true only for lasers, but is a myth otherwise. We concluded that the recombination losses in HBTs would be remarkably small ($\leq 1\%$) and even in solar cells would be tolerable (a few percent) The only truly serious problem might be a degradation in collector breakdown characteristics in HBTs. Available experimental data are in tentative agreement with this conclusion.

C. Publications resulting from this Research Project

1985		Type
1	"Molecular Beam Epitaxial Growth of GaAs on Si (211)," by P. N. Uppal and H. Kroemer, J. Appl. Phys., Vol. **58,** pp. 2195-2203, Sept. 1985.	Journal
1986		
2	"Summary Abstract: Growth of device-quality GaAs and (Al,Ga)As on (211)-oriented silicon substrates, with thin (0.1µm) superlattice buffer layers," (by P.N. Uppal and H. Kroemer); J. Vac. Sci. Technol. B, Vol. **4**, p. 641, Mar./Apr. 1986.	Reviewed Abstract
3	"MBE Growth of GaAs on Si: Problems and Progress," Matls. Res. Soc. Symposia Proceedings, Vol. **67**, *Heteroepitaxy on Silicon*, Edited by J. C. C. Fan and J. M. Poate, pp. 3-14 , 1986.	Proceedings (invited)
4	"Defects in GaP film grown on Si (211) by molecular beam epitaxy," (by D. W. Chung, M. Inada, and H. Kroemer), J. Mater. Res., Vol. **1** (#6), pp. 803-810, Nov./Dec 1986.	Journal
1987		
5	"Polar-on-Nonpolar Epitaxy," J. Cryst. Growth, Vol. **81**, pp. 193-204, 1987.	Proceedings (invited)
6	"Sublattice Allocation and Antiphase Domain Suppression in Polar-on-Nonpolar Nucleation," J. Vac. Sci. Technol. B, Vol. **5** (#4), pp. 1150- 1154, July/Aug. 1987. [Proc. PCSI-14; Invited Paper]	Proceedings (invited)
7	"Control of dislocations in GaAs grown on Si(211) by molecular beam epitaxy," (by J. S. Ahearn, P. Uppal, T.-Y. Liu, and H. Kroemer) J. Vac. Sci. Technol. B, Vol. **5** (#4), pp. 1156- 1161, July/Aug. 1987. [Proc. PCSI-14]	Proceedings

8 "The Structure of GaAs/Si (211) Heteroepitaxial Layers, ," (by Z. Liliental-Weber, E. Weber, J. Washburn, T.-Y. Liu, and H. Kroemer) Matls. Res. Soc. Symposia Proceedings, Vol. **91**, *Heteroepitaxy on Silicon* II, Edited by J. C. C. Fan and J. M. Poate, pp. 91-98, 1987. — Proceedings

1988

9 "Polar-on-Nonpolar Epitaxy: Progress and New Problems," *Gallium Arsenide and Related Compounds 1987*, Inst. Phys. Conf. Ser., Vol. **91**, pp 21-26, 1988. — Proceedings (Invited)

10 "Rotational slip in III-V heterostructures grown by molecular-beam epitaxy," (by M. D.Lind, G. J. Sullivan, T. Y. Liu, and H. Kroemer) J. Appl. Phys., Vol. **64** (#5), pp. 2746-2748, Sept. 1988. — Journal

11 "Luminescence of GaAs/(Al,Ga)As superlattices grown on Si substrates, containing a high density of threading dislocations: Strong effect of the superlattice period," (by T.-Y. Liu, P. Petroff, and H. Kroemer), J. Appl. Phys., Vol. **64** (#12), pp. 6810-6814, Dec. 1988 — Journal

1989

12 "GaAs on Si, and Related Systems: Problems and Prospects," (by H. Kroemer, T.-Y. Liu, and P. M. Petroff), J. Cryst. Growth, Vol. **95**, pp. 96-102, Feb. 1989. (Proc. 5-th Internat. Conf. Molecular Beam Epitaxy, Sappor, Japan, August 1988. Note: Much of the material in this paper was presented already in July 1987, as an Invited Paper at the 7th American Conference on Crystal Growth, Monterey, CA) — Proceedings (Invited)

13 "Electronic Properties of Dislocations in Heavily Dislocated Quantum Well Structures: Doping Effects," (by T.-Y. Liu, P. Petroff, and H. Kroemer), Matls. Res. Soc. Symposia Proceedings, Vol. **145**, *III-V Heterostructures for Electronic/Photonic Devices*, Edited by C. Tu, V. D. Mattera, and A. C. Gossard, pp. 393-398, 1989. — Proceedings

D. Participating Scientific Personnel, and Advanced Degrees earned by them under this Research Project.

Professor H. Kroemer, Principal Investigator:
Throughout entire contract.

Professor Pierre Petroff:
Professor Petroff supervised all electron microscopy done under this contract, which included part of the supervision of the Ph.D. dissertation of Mr. Liu (see below), without formally charging time to this contract, except for one month in the summer of 1989.

Dr. Jim Gaines, Post-Doctoral Research Associate:
Spring 1987 through September 1989; partial support. Balance of support from ONR.

Dr. Parvez Uppal, Post-Doctoral Research Associate:
Fall 1985.

Mr. Tak-Yu Liu, Graduate Research Assistant:
Throughout entire contract.
In September 1990, Mr. Liu received his Ph. D. for this research.

Mr. Dan Leonard, Graduate Research Assistant:
Fall of 1989 and Spring of 1990.